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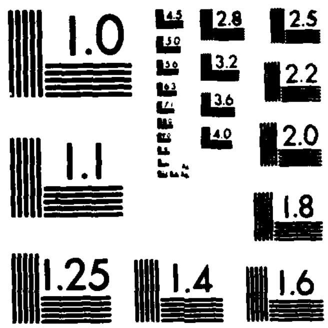

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DIRECT NUMERICAL SIMULATIONS OF THE PDF'S OF A PASSIVE SCALAR IN A FORCED MIXING LAYER

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Abstract - The probability density functions of a passive scalar quantity are calculated in a perturbed mixing layer by means of direct numerical simulations. The results indicate that the two-dimensional rollup of the unsteady shear layer, and the pairing process in particular, contributes greatly to the generation of the predominant peak of the PDF's within the mixing region.

Key Words - Direct Numerical Simulation, Mixing Layers, Probability Density Functions, Coherent Structures, Entrainment.

INTRODUCTION

Probability Density Functions (PDF's) have proven very useful in the theoretical treatment of turbulent reacting flows since the early work of Hawthorne et al. (1949). An approach based on the solution of a transport equation governing the probability density function of the scalar quantities has the advantage that it provides a complete statistical description of all the scalars (Pope, 1979). Therefore, the effects of chemical reactions appear in a closed form eliminating the need for any turbulence modeling associated with the scalar fluctuations. However, models are needed for the closure of the molecular mixing term and also the turbulent convection (O'Brien, 1981).

In most of the previous work employing the PDF approach, the effects of molecular mixing have usually been modeled by using different stochastic models originating from the same "family" of the coalesence-dispersion models (Pope, 1982), whereas simple gradient-diffusion approximations have been employed for the closure of the turbulent flux of the PDF (Givi et al., 1984).

Among these previous works, Givi et al. (1985) used a Monte Carlo numerical routine for the calculations of a modeled transport equation governing the evolution of a passive scalar PDF in a nonreacting two-stream turbulent mixing layer. The results of the prediction were compared with the experimental data of Masutani and Bowman (1986), which were obtained under similar hydrodynamical conditions. Good agreement between predicted results and the measured data was obtained for the first two moments of the scalar quantity. There was a major difference, however, between the calculated and measured profiles of the PDF's. The experimental results indicated that the apparent functional form of the PDF changes very little across the mixing layer and has an intermediate peak at a fixed "preferred" value of the concentration (although the magnitude of this peak changes as the mixing layer is traversed). This behavior was originally documented in the measurments of Konrad (1976) and Koochesfahani (1984) in the mixing transition and post-mixing transition (Breidenthal, 1981) regions of the layer and indicates that a given mixed fluid concentration has the same probability relative to other mixed fluid concentrations, regardless of the position in the layer. The predicted results, however, indicate that the location of the PDF peak, with respect to the concentration coordinate, changes as the layer is traversed, meaning that the PDF of the mixed fluid concentration varies with the cross stream direction of the layer.

The major reason for this discrepancy, as suggested by Givi et al. (1985) and Masutani and Bowman (1986), is due to the shortcomings associated with the gradient diffusion modeling of the turbulent flux of the PDF and is fairly independent of the modeling of the molecular mixing term (Kosaly and Givi, 1987). In a highly intermittent flow such as a mixing layer, regions of turbulent fluid are interrupted by the presence of nonturbulent surrounding fluid. A simple gradient diffusion model is not expected to accurately account for this discontinuity.

By the use of direct numerical simulations, it is now possible to simulate the mixing layer directly without resorting to turbulence models (Riley and Metcalfe, 1980). Direct numerical simulation refers to the numerical solution of the exact transport equations of turbulent flows by means of very accurate and efficient numerical methods. Transport coefficients are chosen to assure that all relevant flow characteristics are accurately resolved so that no turbulence modeling is required. The results of such simulations can be used to obtain useful information on the statistics of the variables characterizing the structure of the flow, which in turn can be used as a basis for turbulence modeling.

In this communication, the results of direct numerical simulations are used to construct the PDF of a passive scalar quantitiy in a perturbed two-dimensional mixing layer. The profiles of the PDF constructed in this manner are used to address the shortcomings associated with the modeling of the turbulent flux of the PDF in the transport equation governing its evolution.

RESULTS

A pseudospectral numerical code developed by McMurtry et al. (1986) was modified to simulate a two-dimensional temporally evolving mixing layer under the influence of harmonic forcing. The numerical resolution was upgraded from the previously used 64 x 64 grid to 256 x 256 equally spaced Fourier modes. This upgrade was required for better statistical analysis of the data used for constructing the PDF's. The flow is assumed periodic in the streamwise direction and free slip, impermeable boundary conditions are employed at the transverse boundaries. Although, the laboratory splitter plate mixing layers evolve spatially downstream and the numerical simulations evolve temporally, important similarities in the dynamics of these two flows make it useful to study accurate numerical simulations of the temporally growing layers. By simple Galilean transformation, a flow quantity averaged in the streamwise direction can be related to the time average of the same quantity at a fixed location in a splitter plate configuration. These averaged quantitities are dependent on the tranverse coordinate and the time. Again, the inverse Galilean transformation relates time to the streamwise location in a splitter plate configuration. There is one structure within the periodic domain at each time step. Statistical analysis are perfromed by sampling 256 data points in the streamwise direction at each transverse location and at each time step. The presence of periodic boundary conditions allows us to use accurate pseudospectral numerical methods; these methods are discussed by McMurtry (1987) and will not be repeated here.

The flow field is initialized with a hyperbolic tangent mean streamwise velocity profile and perturbations corresponding to the most unstable mode of this profile and the first subharmonic of the most unstable mode. The properties of these modes have been evaluated from linear stability theory (Michalke, 1964). The fundamental mode in the mixing layer produces a single vortex rollup. When the subharmonic is added in, a second rollup, or pairing, can occur.

The normalized initial value of the conserved scalar concentration, f, varies from 0 in the bottom stream to 1 in the top stream, and its shape is approximated by the following functional form:

$$f(x,y,0) = \frac{1}{y_0\sqrt{\pi}} \int_{-\infty}^{y} \exp(-\xi/y_0)^2 d\xi$$

The flow is conveniently characterized by two nondimensional parameters: the Reynolds number, $Re = \Delta U\delta/\nu$, based on the mean velocity difference across the layer, the velocity half width, and the kinematic viscosity; and the Peclet number, Pe = Re Sc, where Sc is the molecular Schmidt number. The values of these two parameters were set equal to 200, so that the scales would be accurately resolved on the 256-256 grid points employed in the numerical simulations. The value of y_o was chosen so that the initial concentration thickness and the initial velocity thickness were identical. The time dependent transport equations governing the hydrodynamical variables (velocities and pressure) and the scalar variable (f) are solved with use of the pseudo-spectral code, the results of which are discussed next.

The contour plots of the conserved scalar variable are shown for the purpose of flow visualization. In Fig. 1, we present the time development of the contours of the variable f at four different computational times. Initially, the perturbation associated with the fundamental mode grows until a time of t* ($t^*=t\Delta u/\delta$) equal to 12, when the first rollup occurs. Proceeding in time results in the diffusion of the core of the vortex and the growth of the subharmonic mode, which expresses itself in the form of a second rollup and the pairing of two neighboring vortices. This second rollup is completed by a time of t*=36. Proceeding further in time results in the diffusion of the vortex core with no additional rollup.

The profiles of the PDF's of the variable f obtained by statistical analysis of the instantaneous values of f are shown in Fig. 2. In this figure, the PDF has been plotted as a function of the instantaneous concentration f, and the cross-stream direction of the shear layer. These PDF's represent conditions at the initial stages of the growth ($t^*=3$) and the final stage after the pairing process is completed ($t^*=36$).

A comparison between the two parts of Fig. 2 reveals the effects of vortex dynamics on the structure of the PDF's. Fig. 2a shows that, at the early stages of the development, before any rollup or pairing has occurred, the PDF's can be simply characterized by two delta functions that are located at $f=0$ and $f=1$, with only a negligible amount of mixed fluid at the mixing core of the layer. This indicates that, at any location in the cross-stream direction, the fluid originates from either the top stream or the bottom stream without any significant amount of mixing in the core. Fig. 2b shows that after the occurance of the rollup and the completion of pairing, a third spike appears in the profiles of the PDF at a region in the neighborhood of a concentration value of 0.5. The presence of this third peak suggests the existence of a preferred mixed fluid concentration equal to 0.5. The combined effects of vortex rollup and diffusion are to engulf fluids from the two streams and mix them in the cores of the vortices. As the layer is traversed, the preferred value of this concentration does not seem to change considerably and remains in close proximity to $f=0.5$.

The trimodal shape of the PDF is consistent with that observed experimentally (Koochesfahani, 1984). However, the experimental measurements were performed in the transition and post-transition regions of the mixing layer, whereas the numerical data presented here resulted strictly from a two-dimensional simulation. This indicates that the two-dimensional rollup of the unsteady shear layer can be considered as one possible mechanism by which the third peak is generated in the PDF profiles.

It should be mentioned that the presently calculated third peak of the PDF at the preferred mixed fluid concentration of $f=0.5$ is less pronounced than that observed experimentally by Masutani and Bowman (1986). This may be due to the fact that in the present calculations, the effects of random turbulent motion, which can further enhance mixing, are not taken into account. In order to consider the contributions of turbulent motion into the generation of the third peak in the PDF profile, three-dimensional simulations are required. Furthermore, the asymmetry of the mixing mechanisms, which has been both experimentally (Koochesfahani et al., 1985; Koochesfahani and Dimotakis, 1986; Mungal and Dimotakis, 1984) and numerically (Givi and Jou, 1987) observed for spatially evolving flows cannot be represented in the temporal simulations presented here. The asymmetric mixing mechanism results in a preferred concentration value that is closer to that of the high speed stream and may depend on the ratio of the free stream velocities (Dimotakis, 1986). In the present temporal simulations, the ratio of the magnitude of the free stream velocities is equal to unity and the structure of the flow is symmetric with respect to the streamwise coordinates (as shown by the symmetry of the PDF's with respect to the location $(f,y)=(0.5,0)$ in Fig. 2). Therefore, the numerical simulations cannot predict any other than the arithmatic average of the concentration values of the two streams (i.e., 0.5). Nevertheless, the results indicate that the rollup of the unsteady shear layer contributes greatly to the generation of the predominant peak of the PDF's. The exact role of the small scale turbulence motion on the enhancement of such generation requires full three-dimensional simulation and is the subject of our future research.

Finally, the reason that the methods based on simple gradient diffusion modeling of the turbulent flux of the PDF, such as that employed by Givi et al. (1985), cannot predict the trimodal shape of the PDF obtained in the present simulation is due to the fact that such methods do not consider the influence of intermittency caused by the large coherent structures in the formulation. The results of the direct numerical simulations reported here indicate the importance of such structures in the mixing region of the shear layer and suggest the need for better turbulence models in order to accurately predict the mechanisms of mixing and entrainment in such flows.

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FIGURE CAPTIONS

Figure 1: Plot of the Conserved Scalar Variable (f) Contours at Four Different Computational Times. Contour Minimum is 0, Contour Maximum is 1, Contour Interval is 0.1. (a) $t^*=3$, (b) $t^*=12$, (c) $t^*=24$, (d) $t^*=36$.

Figure 2: PDF's of the Conserved Scalar Variable (f) at Points Across the Mixing Layer Width. (a) $t^*=3$, (b) $t^*=36$.

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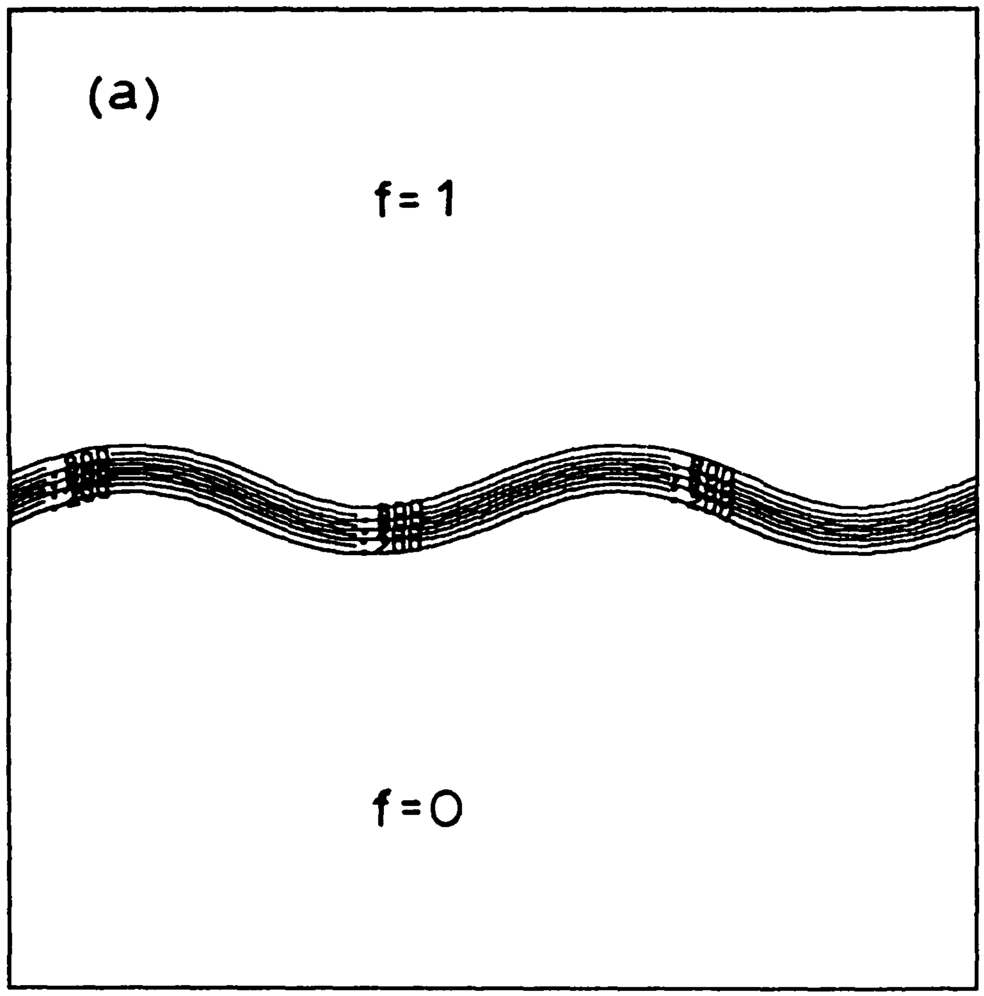

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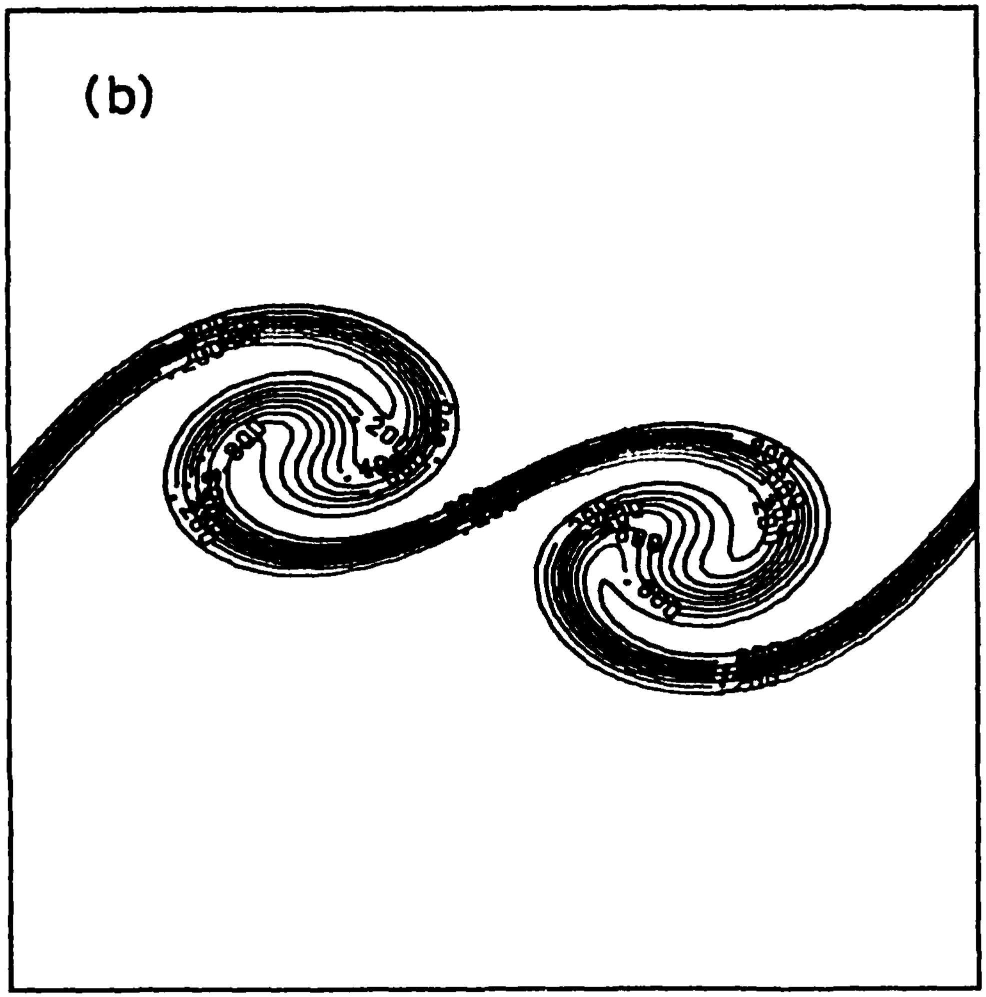

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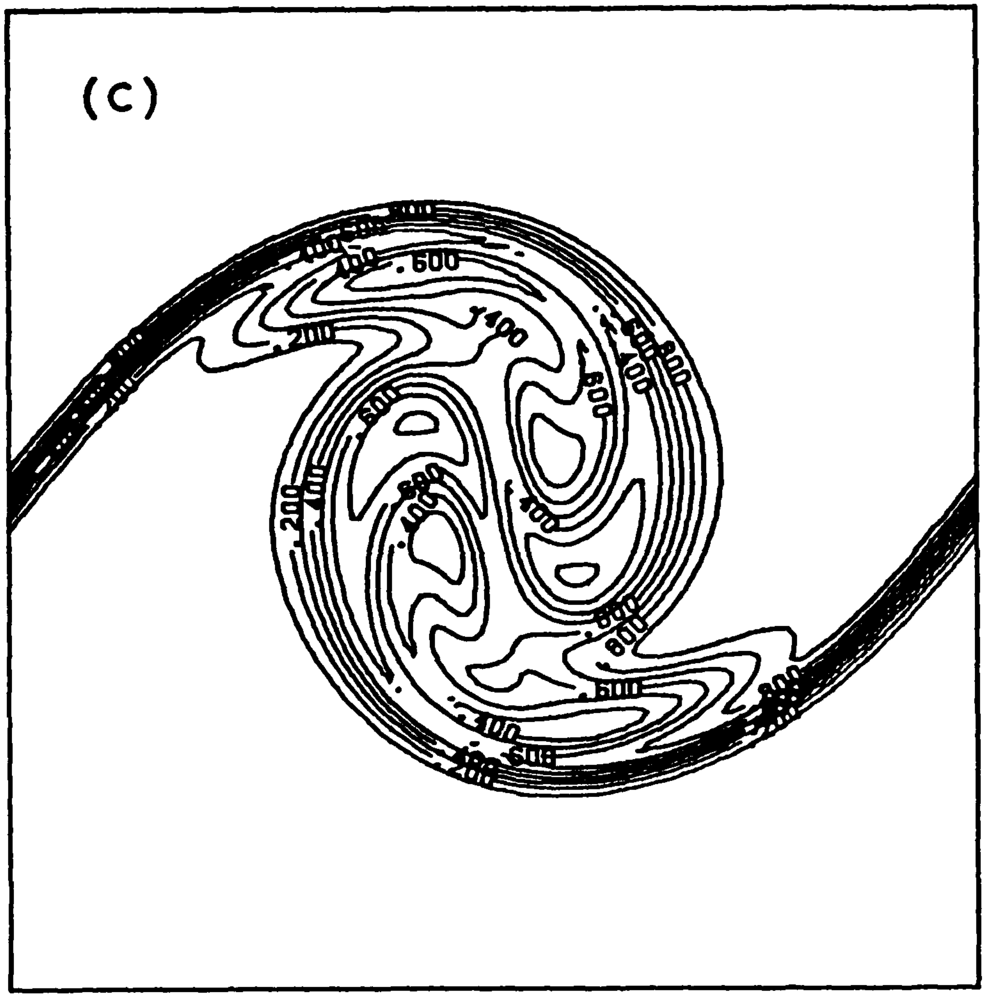

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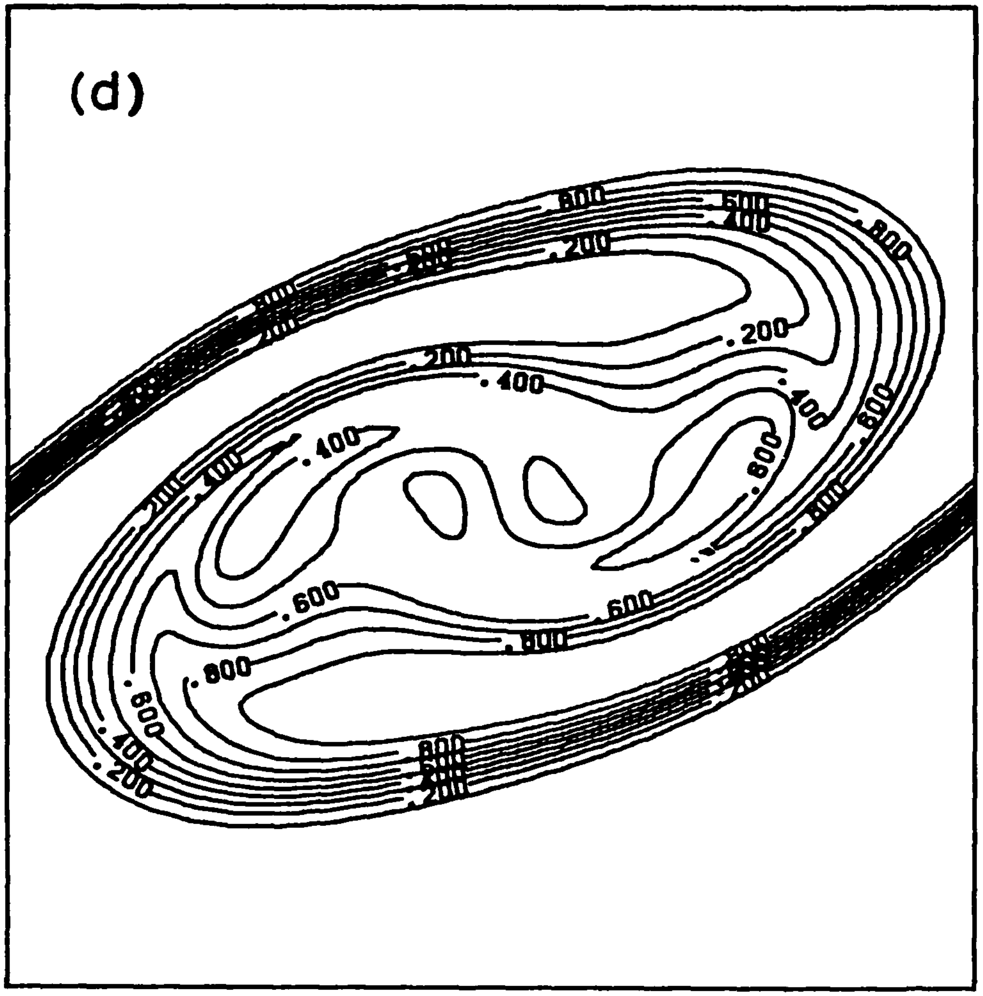

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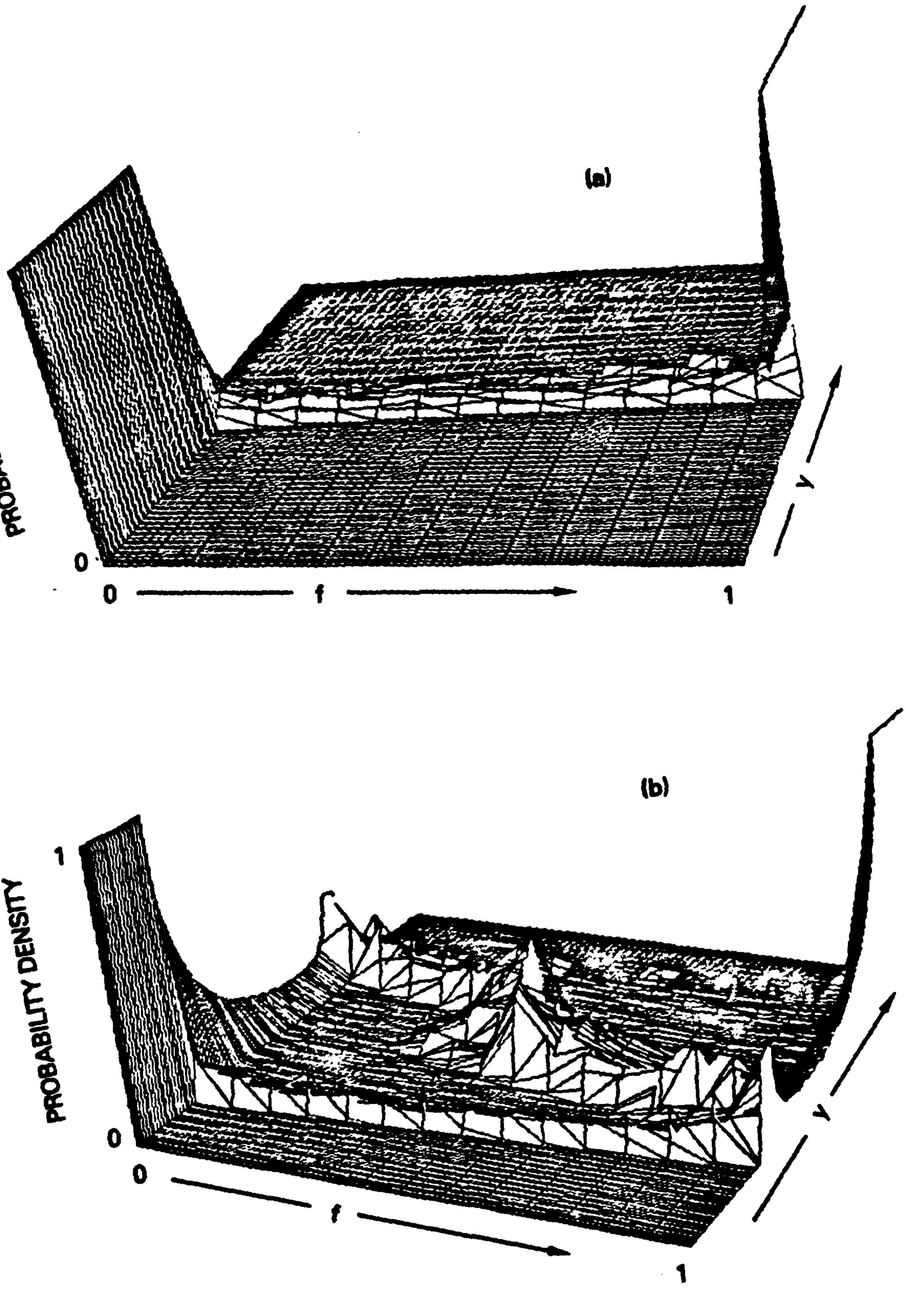
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Figure 2

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